

XINXIN LIU (SHUNSUM LAU)

Master's Student in Physical Chemistry

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EDUCATION

MSc in Physical Chemistry

MOE Key Laboratory of Theoretical Chemistry of Environment;
School of Environment, South China Normal University

2022 – 2025

Guangzhou, China

CGPA: 3.99/5.00

BSc in Applied Chemistry

College of Materials and Energy, South China Agricultural University

2018 – 2022

Guangzhou, China

CGPA: 3.93/5.00

DISSERTATION WORK

MSc Thesis

Relativistic Density Functional Theory Calculations of Molecular
Polarizabilities: Formulation and Implementation

- Reformulated the CPHF/KS approach.
- Extended the CPHF/KS approach to include relativistic two- and four-component methods for analytical (hyper)polarizability calculations of systems with heavy atoms.
- Improved the CPHF/KS approach to support calculations of non-collinear xc functionals.
- Identified three accurate and efficient solvers for the CPHF/KS equations: Krylov subspace, Newton-Krylov, and direct methods.
- Developed a Python code for implementing the above methods in PySCF.
- Research paper of this work is under review in "Physics of Plasmas".

BSc Thesis


DFT Study on the Mechanism of Conversion from Dihydroartemisinin
Acid to Artemisinin

- Proposed a plausible reaction path.
- Identified the initial dominant conformations using xTB.
- Computed the thermochemical data using Gaussian.
- Determined the rate-determining step of the reaction to optimize conditions for drug production.


CERTIFICATES

- CET-6 Certificate.
- NCRE-2 Certificate.
- the **Second Price Award** in the Preliminary Round of the 2019 "FLTRP-ETIC Cup" English Writing Contest.

HOBBIES

 **Exploring Nature and the World**
Observing the nature of things

 **Music Enthusiast**
Enjoying quality music across various genres

 **Reading and Lifelong Learning**
Pursuing continuous learning and meaningful discussions


LOOKING FOR


"To work in a progressive and dynamic research organization where one could solve scientific enigmas and contribute towards welfare of society"

TECHNICAL STRENGTH

| | |
|-----------|-----------|
| Fortran | ● ○ ○ ○ ○ |
| C/C++ | ○ ○ ○ ○ ○ |
| Python | ● ● ● ● ○ |
| Bash | ● ● ○ ○ ○ |
| Tex | ● ● ● ○ ○ |
| Git | ● ● ● ○ ○ |
| MS Office | ● ● ● ● ○ |

MOST PROUD OF

 **Top Performer in College**
Secured 1st position in college in diploma of physical chemistry

 **Knowledge Evolution**
Going next level everyday by perpetual learning of technical and scientific knowledge

STRENGTHS

Thermodynamics & Statistical Mechanics

Linear Algebra

Quantum Mechanics

Calculus

Electrodynamics

Theoretical Mechanics

Careful and Earnest

Hard-working

Flexible and Adaptable

LANGUAGES

| | |
|--------------------|-----------|
| Chinese (Mandarin) | ● ● ● ● ● |
| Cantonese | ● ● ● ● ○ |
| English | ● ● ● ● ○ |
| Japanese | ● ○ ○ ○ ○ |